Multi-Band Semiconductors Synthesized for High Efficiency Solar Cells

Theory Suggests that Conversion Efficiencies Surpassing 50% Are Possible

A team of researchers led by Kin Man Yu and Wladek Walukiewicz in the Electronic Materials Program of the Materials Sciences Division has synthesized a new semiconductor material with multiple energy gaps. Such a material might allow the fabrication of ultra high efficiency solar cells. This type of multiband semiconductor had been theoretically predicted but never before made.

The power conversion efficiency limit for a solar cell employing a single semiconducting material is 31%. The primary basis of this limit is that no single material can absorb light across the full range of solar radiation, which has usable energy in the photon range of 0.4 – 4 eV (infrared to ultraviolet). Light with energy below the bandgap of the semiconductor will not be absorbed and thus not be captured for energy conversion. Light with energy above the bandgap will be absorbed, but the excess energy above the bandgap will be lost in the form of heat. Decades of research in developing single-material solar cells has led to cell efficiencies close to the theoretical limit; the best cell of this type has an efficiency of 25.1%.

One approach to obtaining higher efficiencies involves using stacks of semiconductors, each with a different band gap. In this design, the higher gap materials capture higher energy photons, but do not absorb lower energy photons which then pass through to the lower gap materials (MSD Highlight 02-8). These cells have been demonstrated to have efficiencies of of up to 35%. In the mid-1970s it was predicted that even higher ultimate efficiencies could be realized if the materials themselves had multiple energy gaps. However, no material of this type had ever been synthesized.

The key to producing such a multiband material lay in basic research that developed an understanding of the properties of so-called "highly mismatched alloys" (HMAs, MSD Highlight 99-4). HMAs are compound semiconductors in which a small fraction of the anions are replaced with more electronegative atoms. This alloying produces a material with a new band that can have a strong quantum mechanical interaction with either the occupied valence band or the empty conduction band of the host semiconductor. Using this analysis, it was predicted that a II-VI semiconductor compound for example, (ZnMnTe) in which a small fraction (~1%) of the group VI constituent (Te in this case) is replaced by O could be a multiband semiconductor. However, growth of this material under equilibrium conditions is not possible since the solubility of O in II-VI compounds is too low. This problem was overcome in the successful preparation of substituted II-VI oxide (ZnMnOTe) thin layers by a non-equilibrium synthesis method recently developed at LBNL. In this method the desired amount of oxygen is implanted into a host semiconductor and then the implanted layer is melted by a single laser pulse. Rapid regrowth from the melt traps O atoms into the crystal lattice, forming a thin layer (200 nm thick) of, in this case, homogeneous ZnMnOTe. Optical measurements proved that this new multiband material has two optical transitions at 1.8 and 2.6 eV that are distinctly different from the fundamental band gap transition of the matrix ZnMnTe (2.32 eV).

This new II-VI oxide is the first practical realization of a semiconductor with a narrow intermediate energy band, and thus is a good candidate for the multi-band semiconductors envisioned for high efficiency photovoltaic devices. Theoretical evaluation indicates that a single junction solar cell fabricated from this material can achieve an ideal power conversion efficiency of 56%. Also, it is noted that changing the Mn content or replacing Mn with Mg may provide another way to vary the band structure for further optimization of solar cell performance.

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